



chain nodes :

13 14

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 17 18 19 20 21

chain bonds :

2-13 5-9 13-14

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 17-18 17-21 18-19 19-20  
20-21

exact/norm bonds :

1-2 1-6 2-3 2-13 3-4 4-5 5-6 5-9 7-8 7-12 8-9 9-10 10-11 11-12 13-14 17-18  
17-21 18-19 19-20 20-21

isolated ring systems :

containing 1 : 7 :

G1:O,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom  
12:Atom 13:CLASS 14:CLASS 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:CLASS